

IDAES
Institute for the Design of
Advanced Energy Systems

Nonlinear Model Predictive Control for Solid-Oxide Electrolysis Cell Systems

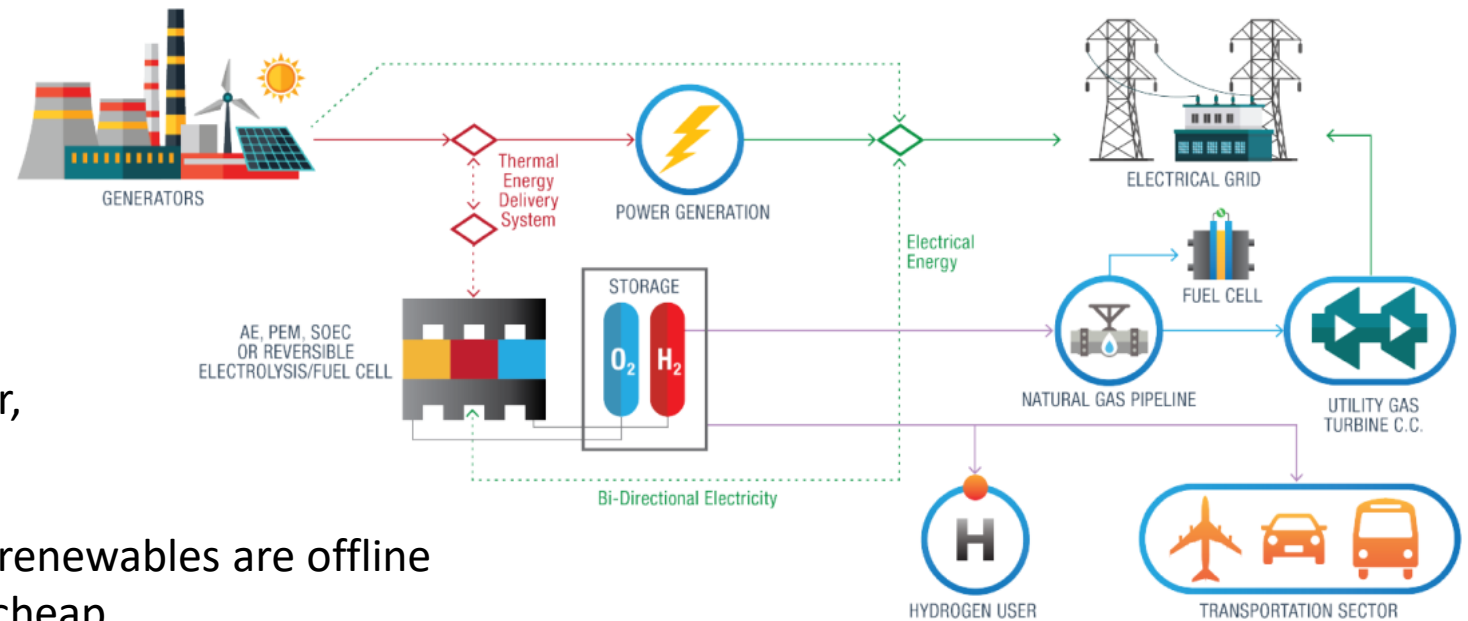
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Tightly-coupled Integrated Energy Systems (IES) play an important role in load-balancing

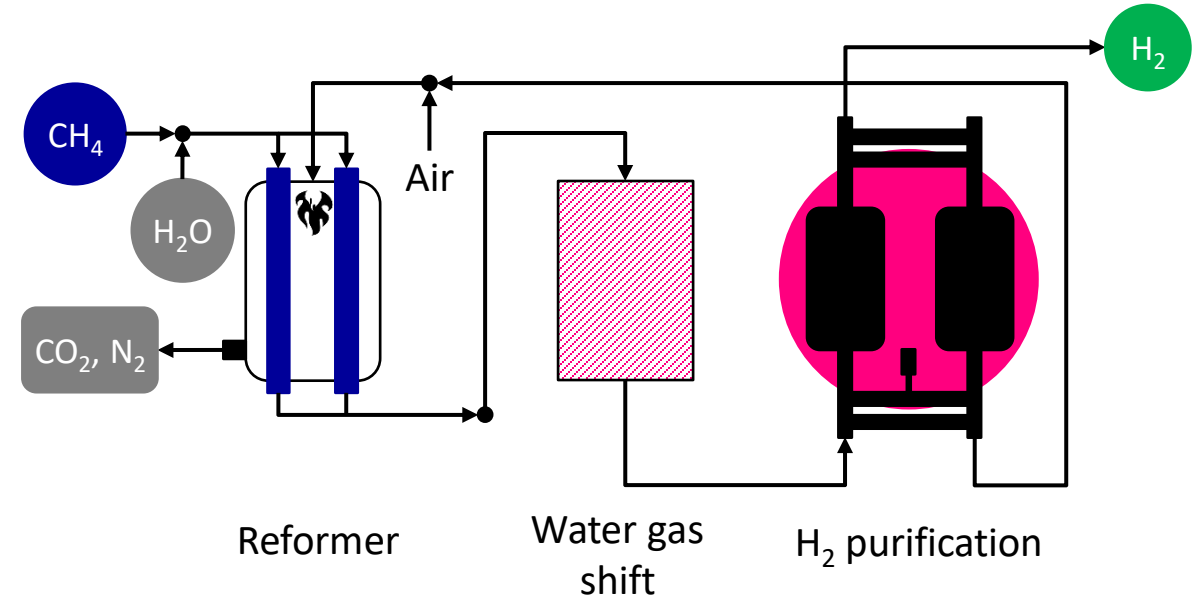
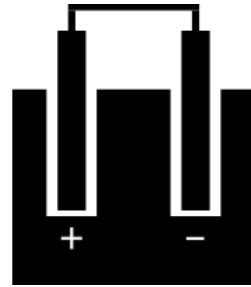
- Intermittent renewable energy adds **volatility to electricity prices**
- IES can **leverage capabilities of diverse energy generators** to provide heat, power, mobility and storage
 - Ramp up electricity production when renewables are offline
 - Produce hydrogen while electricity is cheap



How fast can these systems switch between operating points?

Hydrogen production will play a crucial role in the energy transition and decarbonization

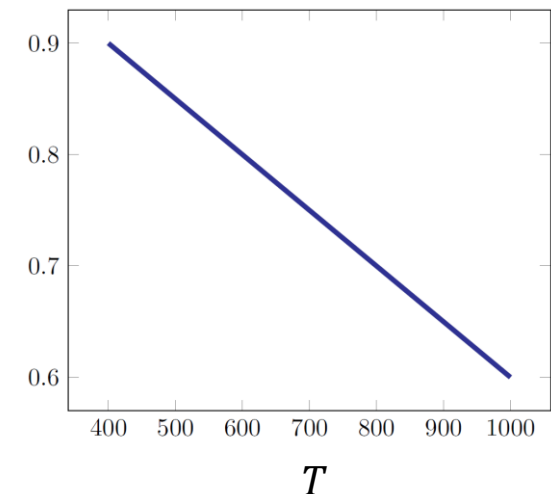
- Most industrial hydrogen is produced through steam-methane reforming, which **uses fossil fuels as feedstock**
- Water electrolysis is a potential replacement, **producing no direct greenhouse gas emissions** when renewable energy is used



- Nernst potential* decreases with increasing reaction temperature

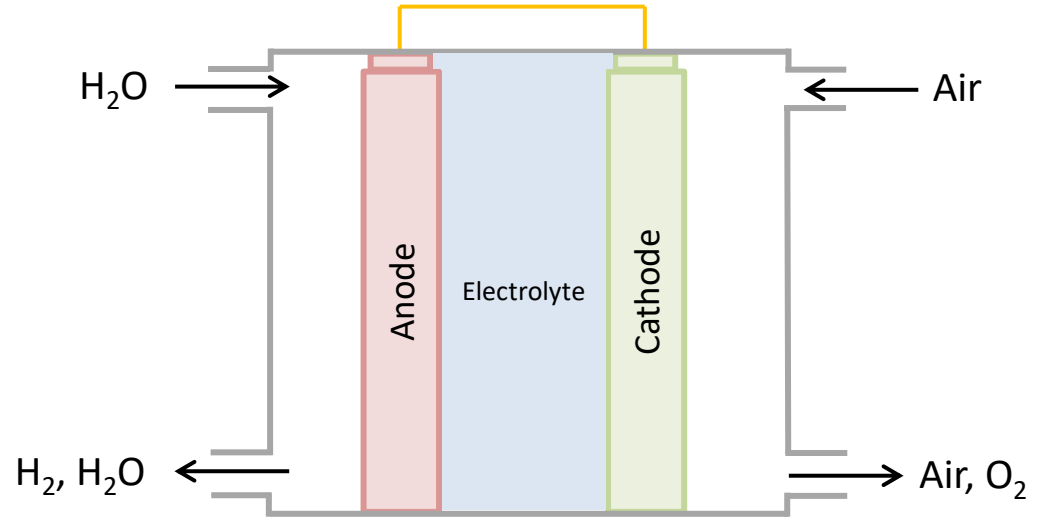
The minimum potential difference at which electrolysis can occur

$$E_{\text{cell}} = E^0 - \frac{RT}{nF} \ln Q$$



Solid-oxide electrolysis cells (SOECs) are candidates for efficient electrolysis

- SOECs operate at 600 °C to 1000 °C, much **higher temperatures** than other electrolysis technologies
- High temperature operation comes with significant drawbacks
 - Additional **heat exchange** equipment
 - Good **thermal insulation**
 - **Careful control** during transition between operating points



Electrolyte: hard, non-porous ceramic material

*Dynamics, health modeling and **advanced process control** are needed to improve SOEC operational performance and thermal management while reducing cell degradation during frequent transients*

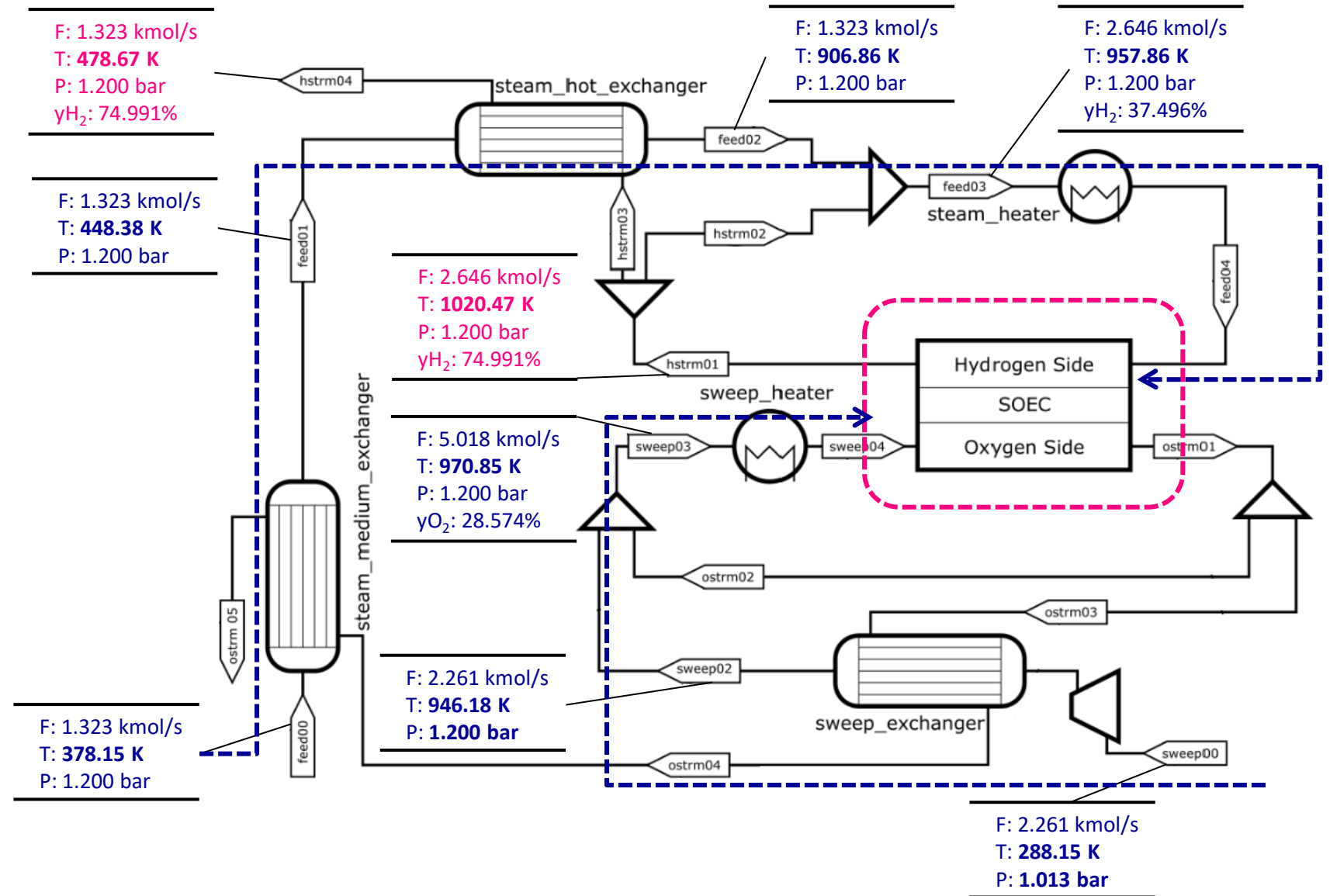
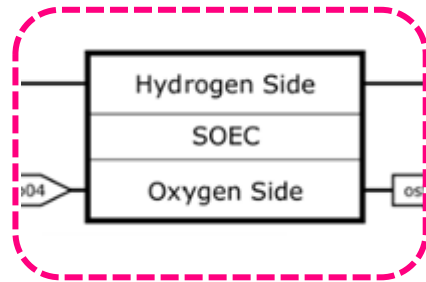
Process flow diagram of SOEC flowsheet



Trim heater



Compressor



Dynamic SOEC modeling as an integration of submodules

Anode (fuel) channel model

$$\frac{\partial C_{i,ac}}{\partial t} = -\frac{\partial}{\partial z} (C_{i,ac} u_{z,ac}) - \frac{J_{i,ac}}{x_{in,an}}$$

$$C_{i,ac} = C_{total,ac} y_{i,ac}$$

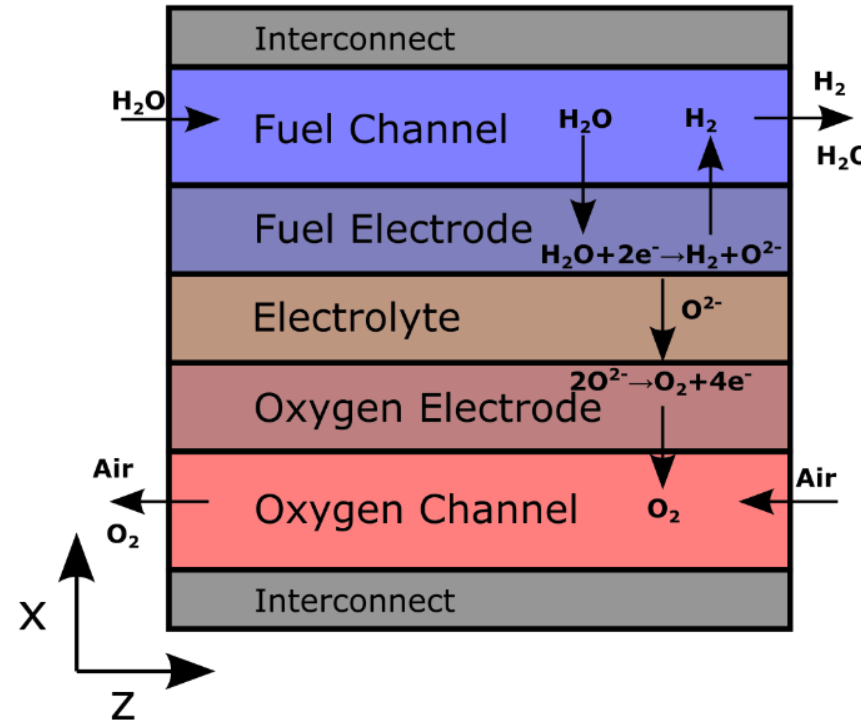
$$C_{total,ac} = f(P_{ac}, T_{ac}, y_{i,ac})$$

$$\sum y_{i,ac} - 1 = 0$$

$$J_{i,ac} = -D_{i,eff} \frac{\partial C_{i,an}}{\partial x} \Big|_{x=x_{in,an}}$$

$$D_{H_2}, D_{H_2O}$$

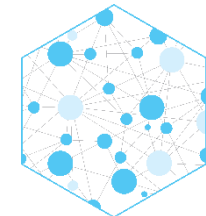
C : molar density, J : flux, D : diffusivity,
ac: anode channel, an: anode, i : species



Nonisothermal, planar SOEC

Fuel electrode: water is reduced into hydrogen

Oxygen electrode: electrode to which O^{2-} ions diffuse



Allan et al. (Under review)

Bhattacharyya et al. (2007)

Dynamic SOEC modeling as an integration of submodules

Anode (fuel electrode) model

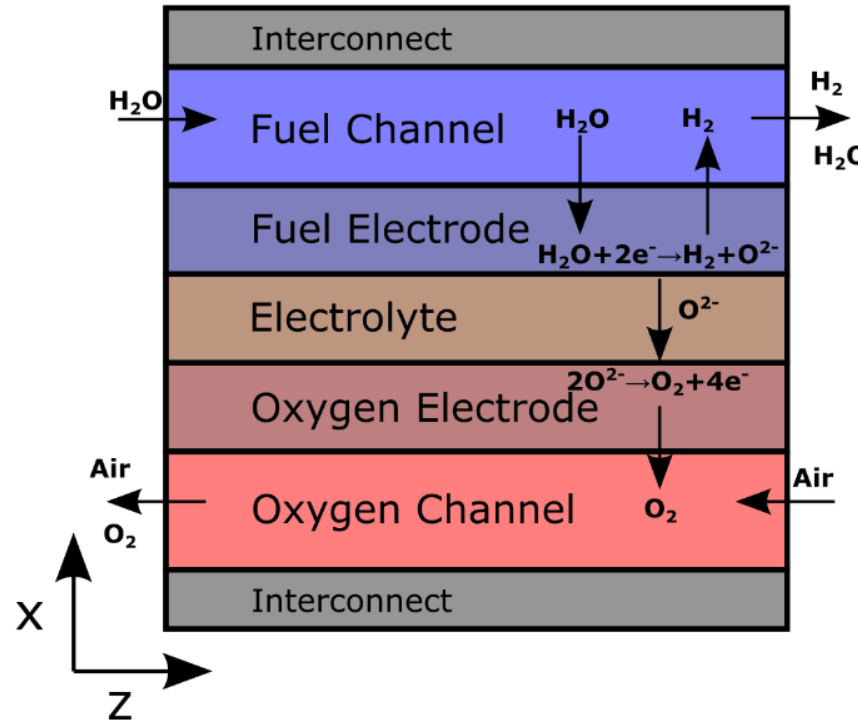
$$\varepsilon_{\text{an}} \frac{\partial C_{i,\text{an}}}{\partial t} = \frac{\partial^2}{\partial z^2} (D_{i,\text{eff}} C_{i,\text{an}})$$

$$C_{i,\text{an}} = C_{\text{total},\text{an}} y_{i,\text{an}}$$

$$C_{\text{total},\text{an}} = f(P_{\text{an}}, T_{\text{an}}, y_{i,\text{an}})$$

$$\sum y_{i,\text{ac}} - 1 = 0$$

C : concentration, J : flux, D : diffusivity,
ac: anode channel, an: anode, i : species



Cathode (oxygen) channel model

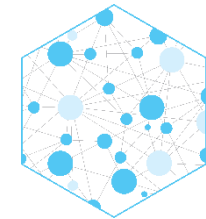
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Cathode (oxygen electrode) model

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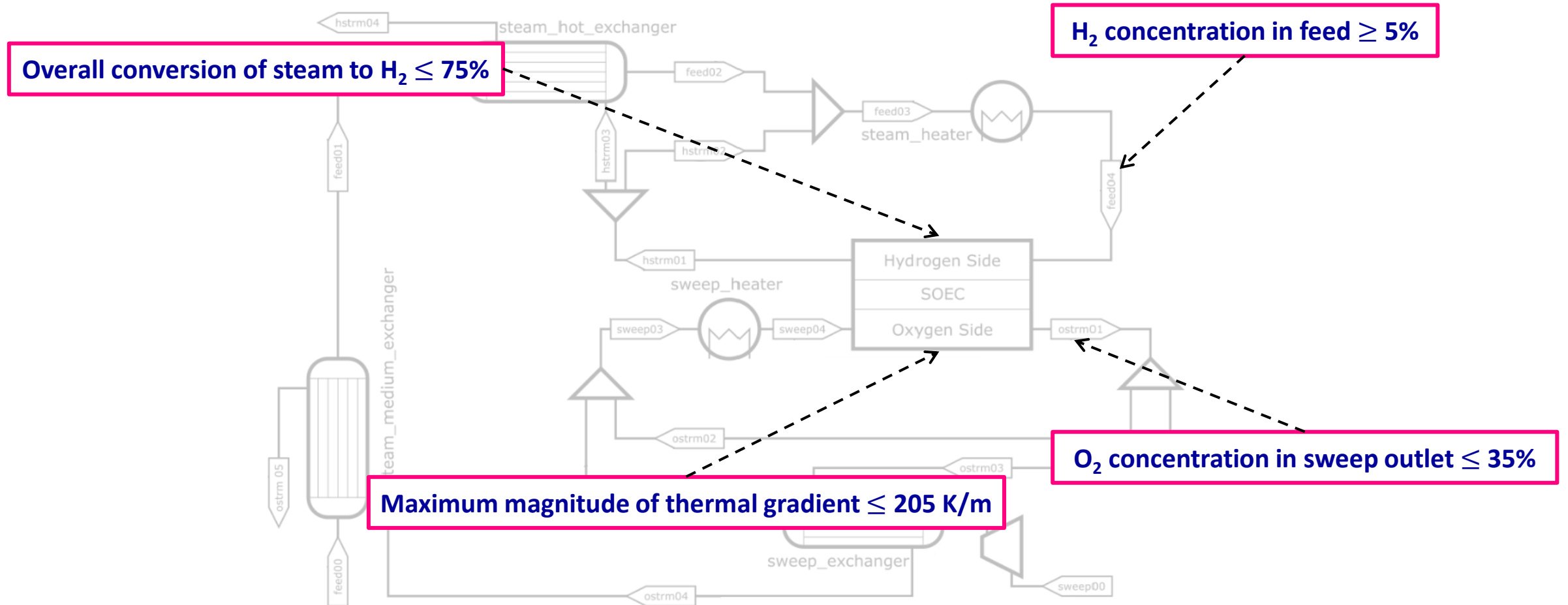
Electrochemical model

- Activation polarization at the cathode and anode
- Ohmic polarization



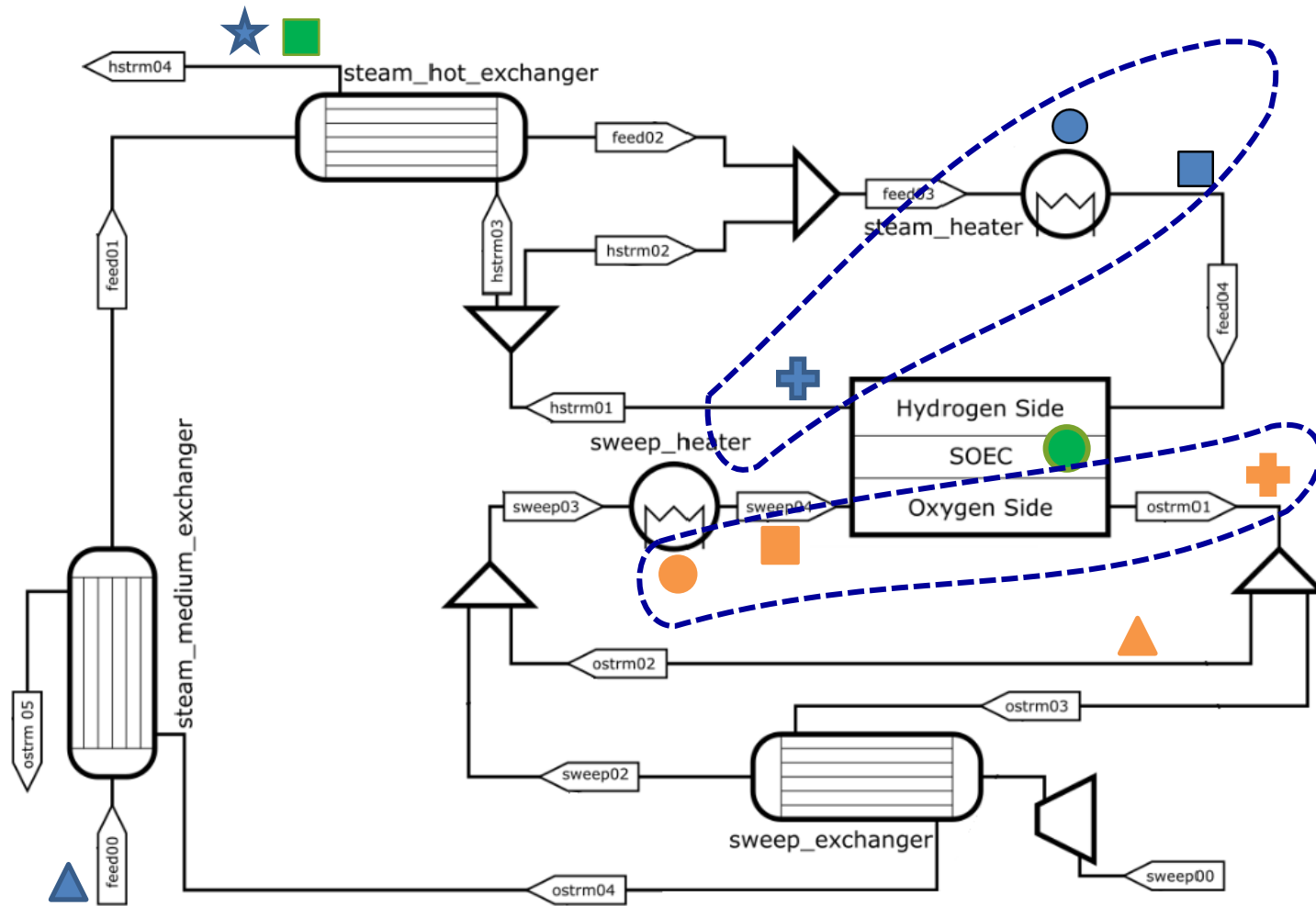
Allan et al. (Under review)

System performance constraints



Transient violations are acceptable

Classical process control pairings



Nonlinear Model Predictive Control (NMPC) can handle highly interactive manipulated variables

NMPC framework developed for setpoint transition using the **same 7 manipulated variables**

$$f_{\text{obj}} = \underbrace{\sum_{i=0}^N \rho_{\text{H}_2} (y_i - y_i^R)^2}_{\text{Trajectory tracking of H}_2 \text{ production rate}} + \underbrace{\sum_{i=0}^N \sum_{j \in J} \rho_j (u_{ij} - u_{ij}^R)^2 + \sum_{i=0}^N \sum_{k \in K} \rho'_k (x_{ik} - x_{ik}^R)^2}_{\text{Deviations of manipulated } (u_{ij}) \text{ and controlled variables } (x_{ik}) \text{ from reference values}} + \underbrace{\sum_{i=1}^N \rho' (\nu_i - \nu_{i-1})^2}_{\text{Rate of change penalties on trim heater duties}} + \underbrace{\rho_s \sum_{i=0}^N \sum_{z=1}^{z_L} (p_{iz} + n_{iz})}_{\ell_1\text{-penalties for temperature gradient constraints}}$$

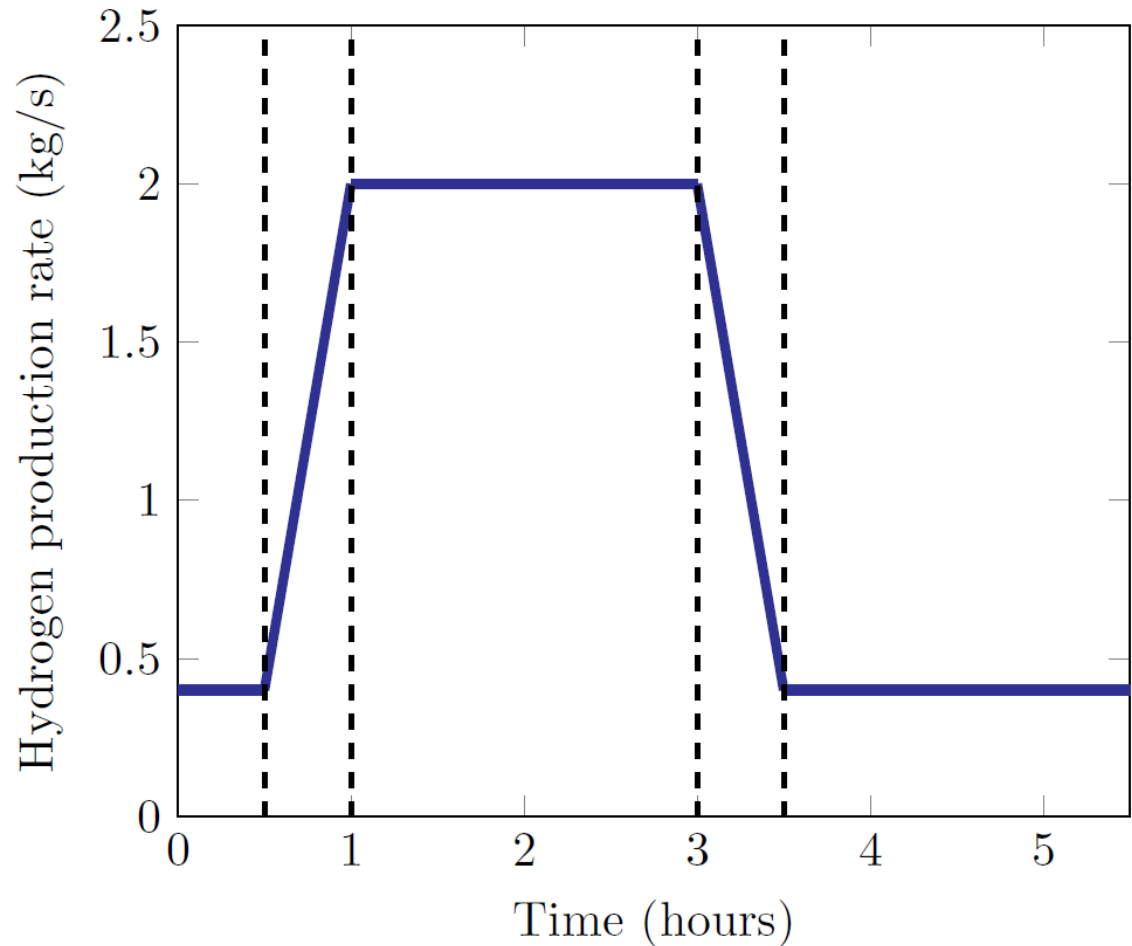
To **prevent thermal degradation** over time, the magnitude of the **temperature gradient** along the cell length (z-direction) is constrained to be below 205 K/m

$$\frac{dT}{dz} - 205 \leq p \quad \text{and} \quad -\frac{dT}{dz} - 205 \leq n$$

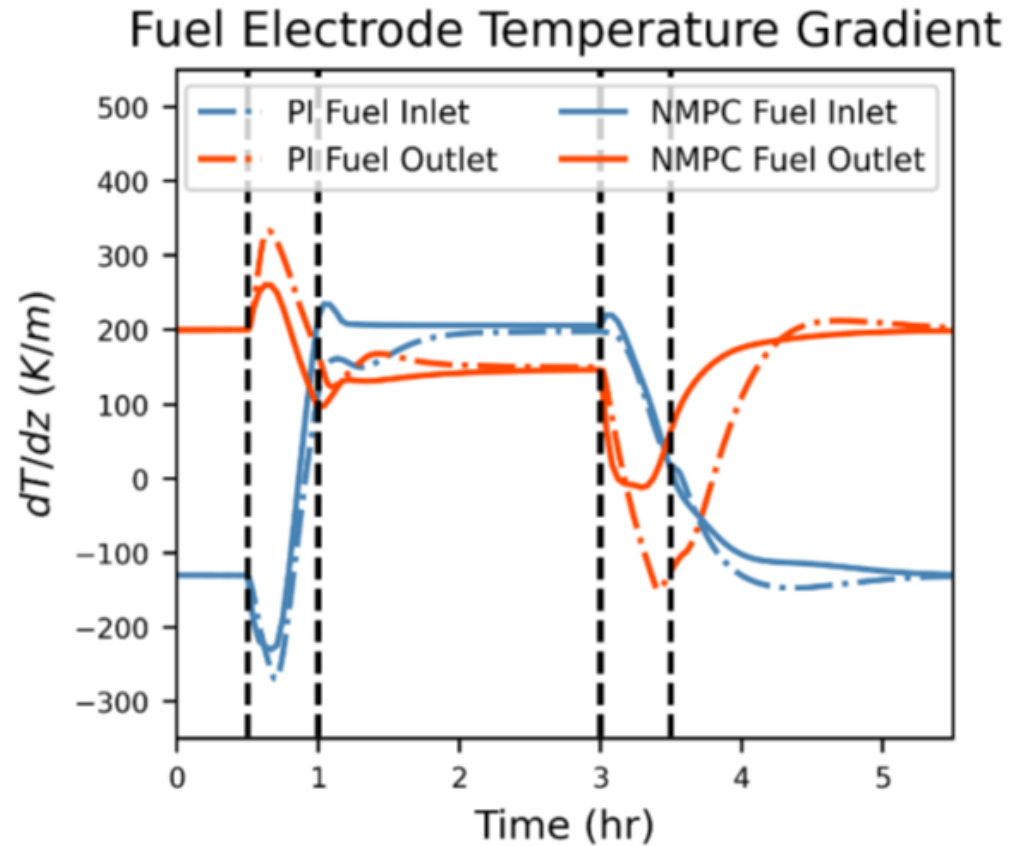
An **ℓ_1 -penalty relaxation** treats them as soft constraints with non-negative slack variables p and n penalized in the objective

Dynamic simulation and control solution approaches to compare classical control with NMPC

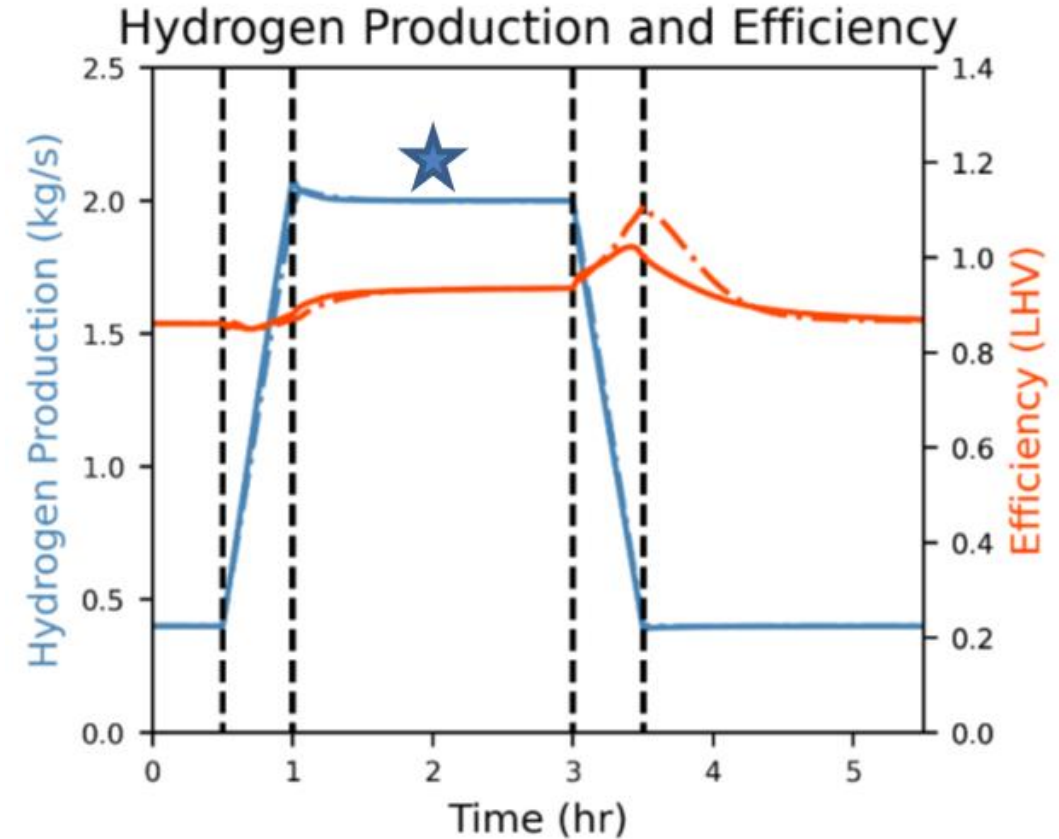
- **Case study: ramp H₂ production**
 - Minimum (0.4 kg/s) to maximum (2.0 kg/s) and back to minimum
 - Each ramp performed over 30 min followed by 2 hrs of settling time
- **Solution approach**
 - Classical: PETSc variable step implicit Euler DAE solver
 - NMPC: **Full-discretization** NLP with IPOPT solver
- **Problem size**
 - Approximately 16000 equations and variables
 - Average solution time of 35.5s for a prediction horizon of 750s



Dynamic simulation and control results



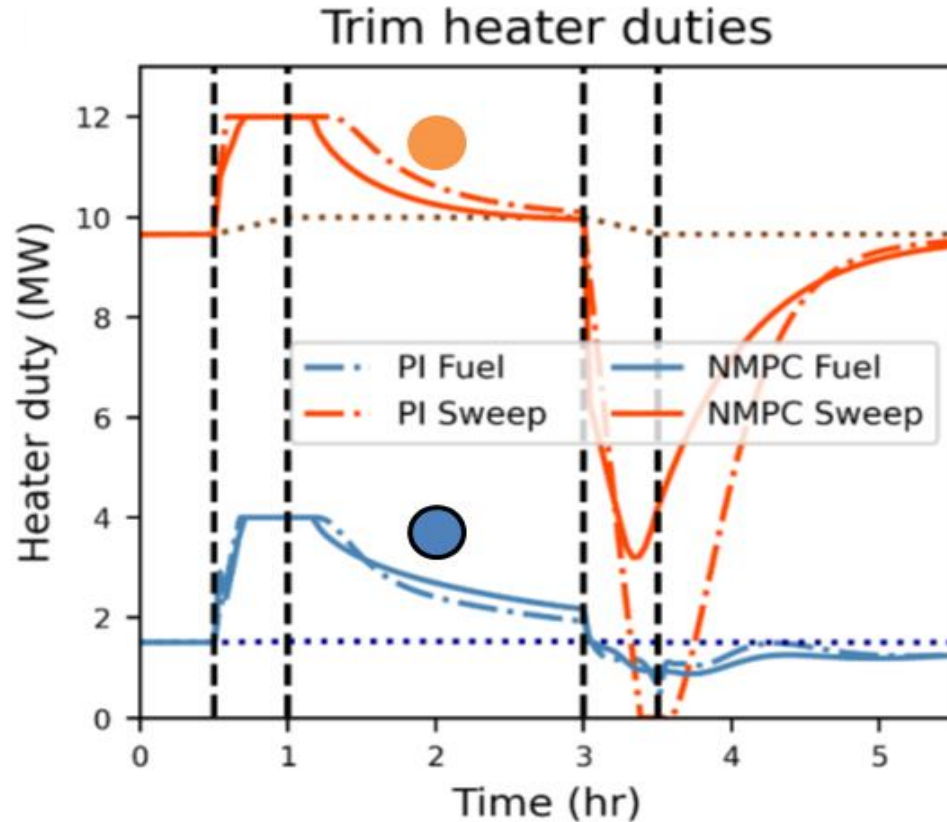
NMPC contains thermal gradients significantly better than sophisticated classical control



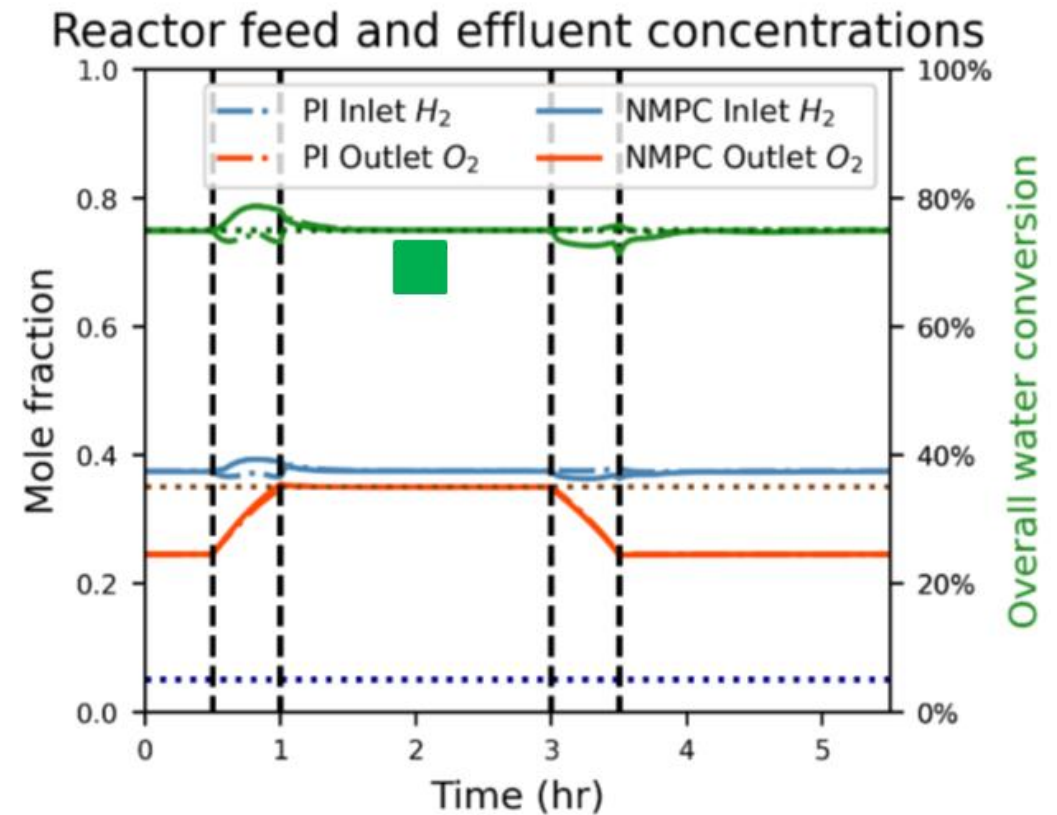
- **Hydrogen production** tracking is identical
- **Efficiency for NMPC is lower** during transients as it takes into account the **restriction of thermal degradation**



Dynamic simulation and control results



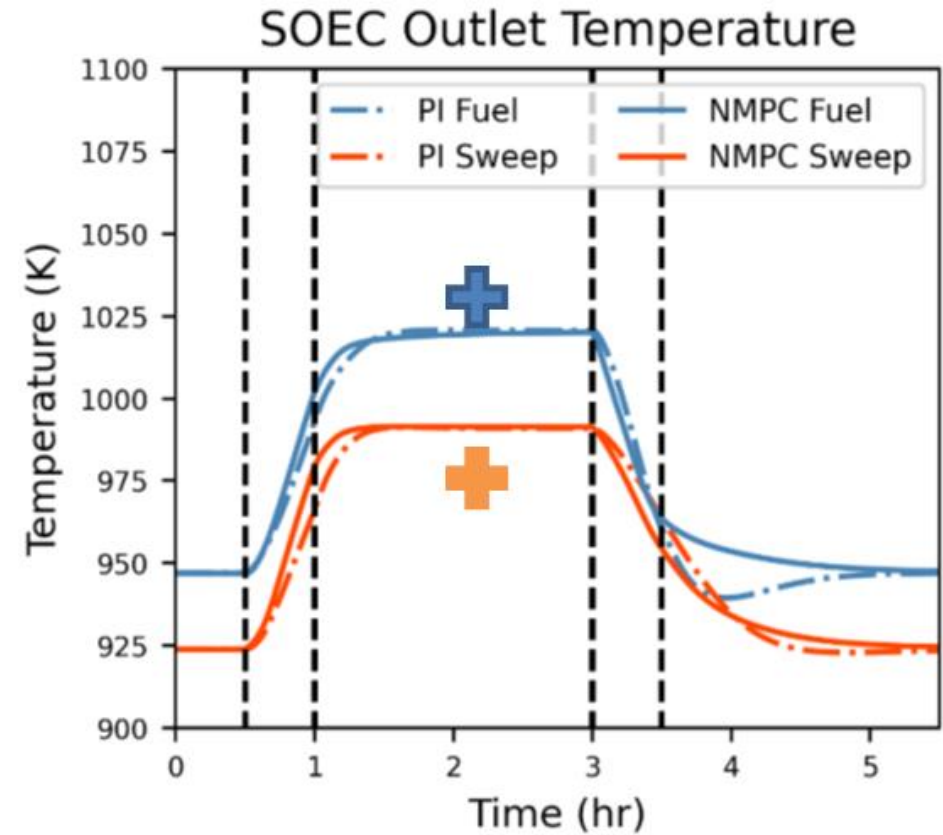
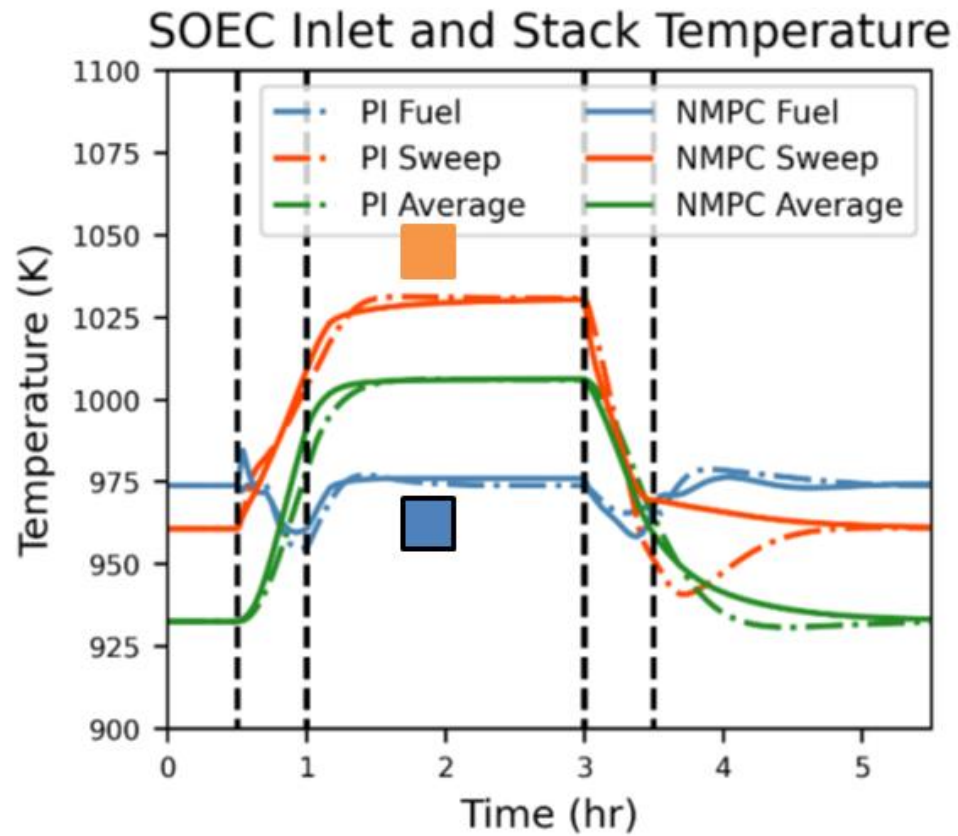
Settling of trim heater duties is faster with NMPC



Performance constraints are satisfied, slight violations during transients



Dynamic simulation and control results



NMPC yields a quicker response in terms of settling of SOEC inlet, outlet and stack temperatures

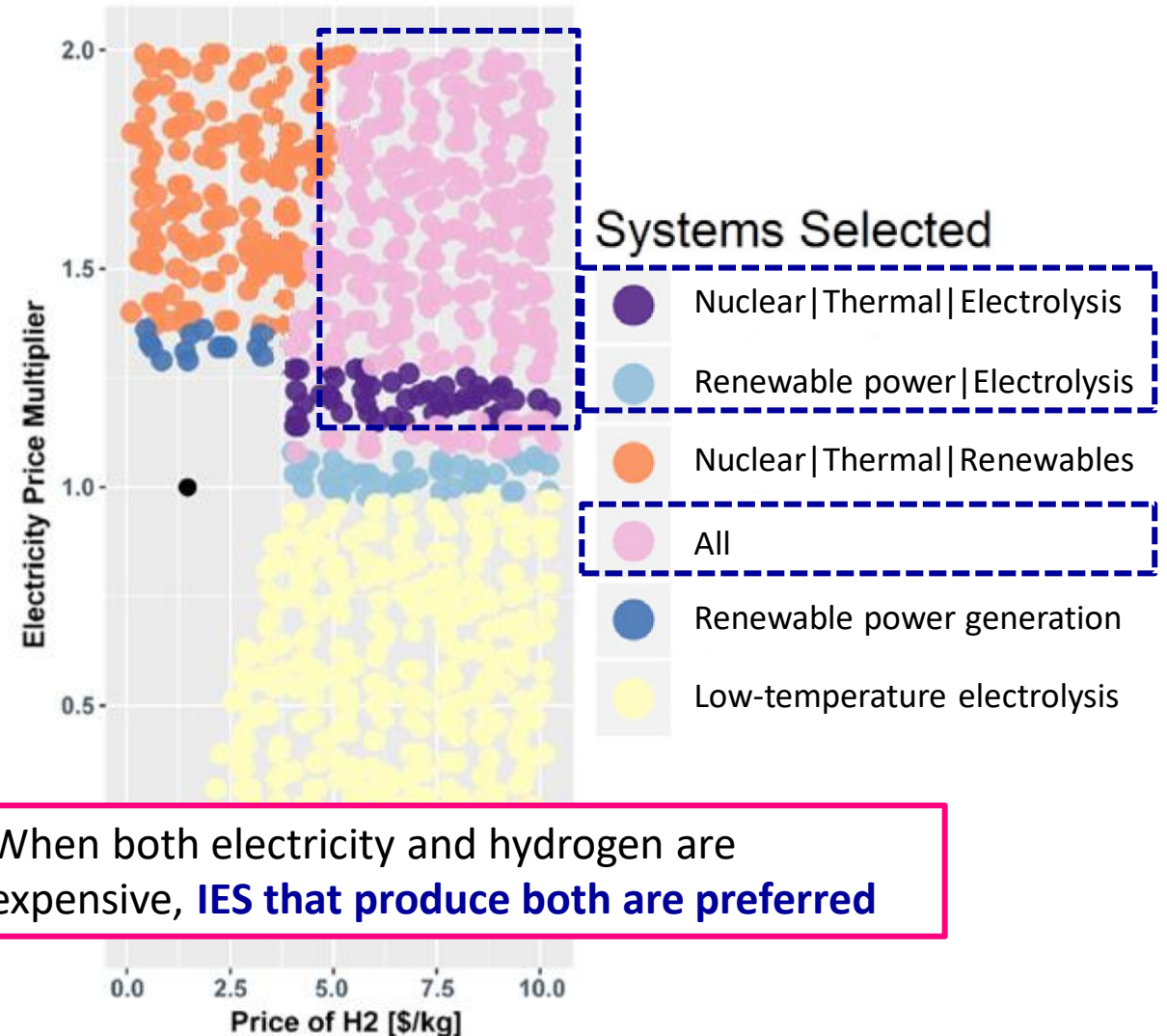


Conclusions, impacts and future directions

- **IDAES offers an ecosystem** of large-scale dynamic models for integrated energy systems, as well as classical and advanced control capabilities
- Setpoint tracking **NMPC can restrict temperature gradients more effectively** compared to classical control
- Matching the tracking performance of NMPC **requires a sophisticated approach** with cascade control – NMPC is suited to handle complex multi-input multi-output systems

Future work

- **Economic NMPC** with more general objective functions
- **Effective mode switching** between hydrogen production and power generation modes



Arent et al. (2021)

idaes.org

github.com/IDAES/idaes-pse



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